

# Pionic Bound States in Momentum Space

Dinghui H. Lu and Rubin H. Landau

Physics Department, Oregon State University, Corvallis, OR 97331

(February 9, 2008)

Bound states of the pion–nucleus system are investigated in momentum space using a microscopic optical potential with inherent energy dependences and nonlocalities arising from elementary potential models. The wave equation and computational techniques are tested, shallow levels are calculated, and a comparison is made with experiment. Deep levels are found to be deeper and broader than those in other investigations.

## I. INTRODUCTION

A complex potential is sometimes used in quantum mechanics to model a physical system which is coupled to another system or channel. This approach is used, for example, in analyzing exotic atoms where an optical potential is added to the Coulomb potential to describe the exotic particle’s strong interaction and eventual annihilation with the nucleus. The normalizable states for such systems are “quasibound” since they decay exponentially in time with a lifetime proportional to the inverse of the imaginary part of the binding energy.

Because strong channel coupling is non perturbative, its phenomenology is often non intuitive. For example, if a potential has sufficiently large imaginary (absorptive) part, an *increase* in the absorptive strength may lead to a *decrease* in the level’s width [1]. Here the increase in the imaginary potential leads to further absorption of the wavefunction from the nuclear interior, and the corresponding decrease in the wavefunction’s overlap with the nucleus leads to a decrease in the level’s width. In these cases, even if the real part of the optical potential is attractive, the large imaginary part acts as a repulsive potential by excluding the wavefunction from the nucleus.

Recently, theoretical studies by Friedman and Scoff [2], Hirenzaki et al. [3], and Toki and Yamazaki [4,5] have pointed out that for deeply bound levels in heavy nuclei, the pion optical potential might be sufficiently absorptive for there to exist states of the type just described. Furthermore, these quasibound states would also be “quasistable” (and thus observable) since their widths would be smaller than the surrounding energy–level spacings ( $\Gamma \simeq \Delta E/10$ ). For example,  $^{208}\text{Pb}$  would have  $1s$  and  $2p$  levels bound by  $\sim 7$  and  $\sim 5$  MeV and widths  $\simeq 0.5$  MeV — in contrast to the  $\sim 20$  MeV widths expected if lowest–order perturbation theory were valid. Furthermore, although the pion is close enough for it to get bound up with the nucleus, the absorption so excludes the wavefunction that the states become hybrid Coulomb–nuclear ones with the dominant binding arising from the Coulomb potential, and the probability density peaking just outside the nuclear surface.

Observing deeply bound pion states in heavy nuclei is difficult because the X-ray cascade ends with the pion being absorbed before it reaches the deep levels. Transitions to the  $1s$  level are seen experimentally only for  $Z < 12$  and to the  $2p$  level only for  $Z < 30$ , and so alternative observational methods have been proposed. A recent experimental search using the  $(n, p)$  transfer reaction did not record the distinct peaks expected for a  $1s$  or  $2p$  transition in Pb [6]. Apparently, the cross sections are smaller, the widths larger, or the binding energies less certain than predicted. Other suggested experiments include  $(n, d)$  pickup [7],  $(\pi^-, \gamma)$  radiative trapping [8], and  $(\pi^-, p)$  pickup [9].

The calculations of deeply bound pion states generally use a phenomenological, coordinate space, optical potential of the Ericson-Ericson form:

$$V^{opt}(r) \simeq \frac{-4\pi}{2\mu} [b_0\rho(r) + c_0\nabla \cdot \rho(r)\nabla + B_0\rho^2(r) + C_0\nabla \cdot \rho^2(r)\nabla] \quad (1)$$

where for clarity we assume here an isoscalar nucleus and leave off the Lorenz–Lorentz factor. The parameters  $b_0, c_0, B_0$ , and  $C_0$  generally are determined by fits to less–bound energy levels in pionic atoms. Because the pion has light mass, relativistic effects are expected to be important, and because the pion has zero spin, the correct dynamical equation is assumed to be the Klein–Gordon equation:

$$[E - V^{coul}(r)]^2 \psi(r) = [-\nabla^2 + \{\mu + V^{opt}(r)\}^2] \psi(r) \quad (2)$$

$$[E - V^{coul}(r)]^2 \psi(r) \simeq [-\nabla^2 + \mu^2 + 2\mu V^{opt}(r)] \psi(r) \quad (3)$$

In (2) the optical potential is treated as a scalar and added to the mass  $\mu$  and the Coulomb potential is treated as the time component of a four–vector and subtracted from the energy  $E$ . Because the square of the optical potential

introduces technical difficulties, the approximation (3) with no  $(V^{opt})^2$  is usually used [2,5,10] (Kwon and Tabakin [11] have indicated how the quadratic term can be handled in momentum space).

The investigation we report upon here was stimulated by the question of how much the properties of deeply bound pionic states would change if a different, possibly more microscopic, form for the optical potential and wave equation were used. In particular, we wondered about using *LPOTT*, the potential we had previously developed for scattering [12,13], but never used for bound states. *LPOTT* is a theoretical optical potential in momentum space having nonlocality, off-shell unitarity, and energy dependence (in addition to its momentum dependence) arising from that of a pi-nucleon  $T$  matrix derived from a separable potential. Since states bound by  $\sim 10$  MeV are quite far down in energy from those at which the constants  $b_0, c_0, B_0$ , and  $C_0$  were fit, we particularly wondered if *LPOTT*'s inherent energy dependence might make a difference. Other factors of interest and difference include finite  $\pi N$  interaction range effects in both the first and second order potentials, covariant kinematics and transformation of scattering amplitudes (“angle transformation”), and the use of the relativistic Schrödinger equation. (Since the relativistic Schrödinger equation is also used in the definition of the  $\pi N$   $T$  matrix and in the derivation of the optical potential, our framework is consistent, which unfortunately, use of (1) in (3) is not.)

In §II we describe the equations and computational method used. In §III A we examine relativistic effects and the numerical precision of our computations, and in §III B make comparisons to the experimental energies and widths of shallow states. Finally, in §III C we examine the deep states supported by our potential, and in §III D deduce what changes in the potential would be needed for there to exist pure nuclear pion bound states. This in turn leads to further understanding of the low energy optical potential.

## II. FORMALISM AND COMPUTATIONAL METHOD

The momentum space relativistic Schrödinger equation is

$$H|\psi\rangle = E|\psi\rangle \quad (4)$$

$$K(k)\psi_l(k) + \frac{2}{\pi} \int_0^\infty V_l(k, k'; E) \psi_l(k') k'^2 dk' = E\psi_l(k) \quad (5)$$

$$\sqrt{m_\pi^2 + k^2} + \sqrt{m_A^2 + k^2} - m_\pi - m_A = K(k) \quad (6)$$

Here  $K(k)$  is the relativistic kinetic energy and  $V_l(k, k'; E)$  is the energy-dependent pion-nucleus potential after partial wave projection. There is no difficulty in momentum space with the square roots in  $K(k)$  since they contain just numbers not operators. Although the relativistic Schrödinger equation (5)-(6) obviously contains relativistic kinematics, it is not covariant. However, it is the direct part of the Blankenbecler–Sugar equation, which is the 3D reduction of the Bethe–Salpeter equation, a covariant, two-particle equation [14,15]. The Klein–Gordon equation, in turn, is relativistic and covariant, but it is only a one-particle equation, and when used as in (3) does not treat the optical potential covariantly.

To handle the most general case of coupled and open channels, we transform (4) to an integral equation involving the Green's function (where the appropriate boundary conditions are incorporated) [16]:

$$|\psi\rangle = G_E V_E |\psi\rangle \quad (7)$$

$$\psi_l(k) = \frac{2}{\pi} \frac{1}{E - K(k)} \int_0^\infty V_l(k, k'; E) \psi_l(k') k'^2 dk' \quad (8)$$

Note that for bound states there is no incident wave in (7) and no  $+i\epsilon$  in  $G_E$ . If we consider  $V_E, K$ , and  $G_E$  as operators or their matrix representation, then we see that solution of the eigenvalue problem (4) is equivalent to demanding nontrivial solutions of (7), namely,

$$(1 - G_E V_E) |\psi\rangle = 0 \quad \Rightarrow \quad \det[1 - G_E V_E] = 0 \quad (9)$$

We search for solutions of (9) in complex energy space after removing the Coulomb singularity with the Lande' subtraction technique. Solving (9) is equivalent to determining the energies of the poles of the  $\pi$ -nucleus  $T$  matrix [16]. In contrast, the momentum space formulations of Kwon and Tabakin [11] and Cieplý et al. [17] directly solve (5) as an eigenvalue problem (Kwon and Tabakin use the Lande' subtraction and Cieplý et al. use the Vincent–Phatak cutoff). In further contrast, Kalbermann et al. [18] sidetrack momentum space entirely and include finite range effects (but not the full energy dependence of a separable  $\pi N$   $T$  matrix), by solving an integro-differential wave equation in coordinate space.

In our calculations, the potential  $V_E$  is taken as the sum of electromagnetic plus optical potentials:

$$\langle \vec{k}' | V_E | \vec{k} \rangle = V^{coul}(\vec{q}) + V^{VP}(\vec{q}) + V_E^{OP}(\vec{k}', \vec{k}) \quad (10)$$

$$V^{coul}(\vec{q}) = -\frac{Z\alpha\rho_p(q)}{2\pi^2q^2} \quad (11)$$

$$V^{VP}(\vec{q}) = -\frac{Z\alpha^2\rho_p(q)}{2\pi^3} \int_1^\infty \frac{(2t^2+1)(t^2-1)^{1/2}}{3t^4(q^2+(2t/\lambda_e)^2)} dt \quad (12)$$

Here the momentum transfer  $\vec{q} = \vec{k}' - \vec{k}$ ,  $V^{coul}$  is the Coulomb potential for a nucleus of finite size,  $\rho_p(q)$  is the proton form factor,  $V^{VP}$  is the order- $Z\alpha^2$  vacuum polarization (Uehling) potential [11,19], and  $\lambda_e$  is the electron Compton wavelength. The optical potential  $V^{OP}$  is evaluated in the impulse and factored approximations, and contains terms of first and second order in  $\rho$ :

$$V_E^{OP}(\vec{k}', \vec{k}) = U_E^{(1)}(\vec{k}', \vec{k}) + U_E^{(2)}(\vec{k}', \vec{k}) \quad (13)$$

$$U_E^{(1)}(\vec{k}', \vec{k}) = Z \langle \vec{k}', \vec{p}_0 - \vec{q} | t_{\omega_{3B}}^{\pi p} | \vec{k}, \vec{p}_0 \rangle \rho_p(q) + N \langle \vec{k}', \vec{p}_0 - \vec{q} | t_{\omega_{3B}}^{\pi n} | \vec{k}, \vec{p}_0 \rangle \rho_n(q) \quad (14)$$

$$= \frac{\gamma}{2\pi^2} \sum_{ilj} \frac{g_{ilj}(\kappa') g_{ilj}(\kappa)}{D_{ilj}(\omega_{3B})} P_l(\cos \theta_{\kappa' \kappa}) \rho_i(q) \quad (15)$$

$$D_{ilj}(\omega) = \frac{1}{\sigma_{ilj}} - \frac{2}{\pi} \int_0^\infty \frac{g_{ilj}^2(\kappa)}{\omega - E_\pi(\kappa) - E_N(\kappa) + i\epsilon} \kappa^2 d\kappa \quad (16)$$

$$U_E^{(2)}(\vec{k}', \vec{k}) = -\frac{4\pi A^2}{2\mu_{\pi A}(2\pi)^3} [B_0(E) \frac{\hat{g}_s(\kappa) \hat{g}_s(\kappa')}{\hat{g}_s^2(\kappa_0)} + C_0(E) \frac{\hat{g}_p(\kappa) \hat{g}_p(\kappa')}{\hat{g}_p^2(\kappa_0)} \vec{\kappa}' \cdot \vec{\kappa}] \rho^2(q) \quad (17)$$

$$\hat{g}_s(\kappa) = \frac{1}{\alpha_s^2 + \kappa^2}, \quad \hat{g}_p(\kappa) = \frac{1}{(\alpha_p^2 + \kappa^2)^2} \quad (18)$$

Here  $ilj$  labels the  $\pi N$  eigenchannel ( $i$  = proton, neutron, or isospin,  $l$  = orbital, and  $j$  = total angular momentum),  $\sigma_{ilj}$  is the sign of the potential in that eigenchannel, and  $\kappa$  and  $\kappa'$  are the initial and final  $\pi N$  COM momenta. The nuclear form factors  $\rho_{p,n}(q)$  in (14) and (17) are Fourier transforms of Woods-Saxon densities [12]. To aide comparison with other optical potentials, we take the size parameters as the standard set used by Friedman et al. [20] with extension to Pb by use of the charge parameters from De Vries et al. [21]. The parameters are given in Table I.

For simplicity of calculation we have used the factored form of  $U^{(1)}$  (14), which clearly does not average over the nucleons' Fermi momenta. We can remove this limitation, yet the computation would be longer, more complicated, and possibly less reliable as we extrapolate deep down in energy. We do include nucleon recoil in part, by making the optimal choice for the momentum of the struck nucleon [13],

$$\vec{p}_0 = -\frac{\vec{k}}{A} + \frac{(A-1)\vec{q}}{2A} \quad (19)$$

This  $\vec{p}_0$  is optimal in producing the best factored approximation and the most physical off-energy-shell kinematics. We include further recoil and Fermi motion effects in our use of the three-body subenergy  $\omega_{3B}$  as the  $\pi N$  energy in (14). This choice arises from a three-body model for the optical potential [13] in which there is a pion of momentum  $\vec{k}$ , a nucleon of momentum  $\vec{p}_0$ , and a core of momentum  $\vec{P} = -(\vec{k} + \vec{p}_0)$ . The  $\pi N$   $T$  matrix is then evaluated at an energy which is the magnitude of the difference in energies of the  $\pi N$  pair and the core:

$$\omega_{3B}^2(E) = (k_\pi^\mu + k_A^\mu - P^\mu)^2 \simeq [E + m_\pi + m_A - E_{A-1}(P) - E_B]^2 - P^2 \quad (20)$$

Here  $E_B$  is an effective core-nucleon binding energy we take as 20 MeV. Changing  $E_B$  to 10 MeV would increase our final  $\Gamma_{1s}(\text{Pb})$  by  $\sim 20\%$ , and  $E_{re}(\text{Pb})$  by  $\sim 1\%$ .

Pauli blocking is included by modifying the  $\pi N$   $T$  matrix for a nucleon embedded in a Fermi sea with Fermi momentum  $P_F$  appropriate to the nucleus in question [13]. Specifically we modify the  $D$  functions in (16) with an angle-averaged Pauli operator  $Q_0$ :

$$D_\alpha(\omega) \rightarrow D_\alpha^{(P)}(\omega) = \frac{1}{\sigma_\alpha} - \frac{2}{\pi} \int_{\xi P - P_F}^{\xi P + P_F} \frac{g_\alpha^2(\kappa) Q_0(P, \kappa)}{\omega - E_\pi(\kappa) - E_N(\kappa) + i\epsilon} \kappa^2 d\kappa \quad (21)$$

$$Q_0(P, \kappa) = \begin{cases} 0, & \xi P + \kappa < P_F \\ 1, & |\xi P - \kappa| > P_F \\ \overline{Q}_0, & \text{otherwise} \end{cases} \quad (22)$$

$$\overline{Q}_0 = \frac{(\xi P + \kappa)^2 - P_F^2}{4\xi P \kappa}, \quad \xi = \frac{m_N}{m_N + m_\pi} \quad (23)$$

The two-body  $T$  matrices and momenta in (14) are related to off-shell ones in the  $\pi N$  COM by a Lorentz covariant prescription [13] which determines  $\gamma$ ,  $\vec{\kappa}$ , and  $\vec{\kappa}'$ . As indicated by the  $g_{ilj}$  product in (14), we include the finite range of the  $\pi N$  interaction by using a separable potential [12] which, in turn, was fit to  $\pi N$  scattering data. Note, the explicit energy dependence given by the solution of the  $\pi N$  T matrix in (14)-(15) is important for the present study of deeply bound states because it permits a physically motivated evaluation of optical potential far below the  $\pi N$  threshold. Since our model has finite range  $\pi N$  interactions, inclusion of a Lorentz-Lorenz term is inappropriate [13,18].

The second order potential  $U^{(2)}$  includes contributions from processes such as virtual nuclear excitation and pion annihilation (true absorption). It is particularly important for pionic atoms since its imaginary part provides absorption. The form we use for  $U^{(2)}$  in (17) is a generalization of the separable form used for  $U^{(1)}$  (we take  $\kappa_0 \rightarrow 0$  for subthreshold extrapolation). Unfortunately, while tremendous theoretical and experimental progress has been made in understanding the contribution of true pion absorption to the pi-nucleus interaction, that progress is not far enough along to permit a determination of  $U^{(2)}$  with enough accuracy for present purposes. Consequently, the quantities  $B_0$  and  $C_0$  are fit to the  $1s$  and  $2p$  levels' shifts and widths in pionic  $^{16}\text{O}$  and  $^{40}\text{Ca}$ . In addition, while for scattering we modeled the energy dependence of  $B_0$  and  $C_0$  as that of the  $\pi^+ D \rightarrow pp$  cross section, we have not been able to determine a reliable, analytic continuation for subthreshold energies using the energy dependence of either  $\sigma(\pi^+ D \rightarrow pp)$  or the parameters of Cieplý et al. [17]. While our estimates indicate that the subthreshold energy dependence is weak, our ignorance of it weakens our model.

Since our solution of (9) determines the complex eigenenergies but not eigenfunctions, once the eigenenergies are known we solve for the momentum space wavefunctions by using inverse iteration [11] on the Schrödinger equation (5):

$$[H_E] [\psi_l(k_i)] = E [\psi_l(k_i)] \quad (24)$$

$$[\psi_l(k_i)] = [H_E - E]^{-1} [\psi_l(k_i)] \quad (25)$$

The wavefunction normalization is then

$$1 = \int_0^\infty \psi_l^2(k) k^2 dk \quad (26)$$

$$\Rightarrow 1 = \int_0^\infty [(\text{Re } \psi_l(k))^2 - (\text{Im } \psi_l(k))^2] k^2 dk \quad (27)$$

$$0 = \int_0^\infty \text{Re } \psi_l(k) \text{Im } \psi_l(k) k^2 dk \quad (28)$$

Note that the normalization condition (26), which follows from the Gamow state formalism of Hernández and Mondragon [22], normalizes the square of the complex wave function rather than the square of the modulus. This in turn requires the overlap of  $\text{Re } \psi_l(k)$  and  $\text{Im } \psi_l(k)$  to vanish (28), which often introduces an oscillation in  $\text{Re } \psi_l(r)$ . Once the momentum-space wavefunction is known, it is transformed to coordinate space via:

$$\psi_l(r) \equiv \frac{u_l(r)}{r} = i^l \left( \frac{2}{\pi} \right)^{1/2} \int_0^\infty \psi_l(k) j_l(kr) k^2 dk, \quad (29)$$

### III. RESULTS AND DISCUSSIONS

#### A. Relativistic Effects and Numerical Precision

Relativistic effects should be important for deeply bound states in heavy nuclei. While our dynamical equation is the relativistic Schrödinger equation (5), in contrast to the more conventional approximate Klein-Gordon equation (3), it

is reasonable to wonder if either equation is adequate for calculating such states. We examine the point Coulomb case since then we know the analytic solutions to the Schrödinger equation (the Bohr energies) and to the Klein–Gordon equation [15,23]:

$$E_{nl}^{KGE} = \frac{mc^2}{\{1 + (Z\alpha)^2/[n - l - \frac{1}{2} + \sqrt{(l + \frac{1}{2})^2 - (Z\alpha)^2}]^2\}^{1/2}} \quad (30)$$

$$\simeq mc^2 - \frac{mc^2(Z\alpha)^2}{2n^2} - \frac{mc^2(Z\alpha)^4}{2n^4} \left( \frac{n}{l + \frac{1}{2}} - \frac{3}{4} \right) + O(\alpha^6) \quad (31)$$

To compare with the two-particle Schrödinger theory, we use a reduced mass  $\mu$  in the second term of (31) and the pion mass  $m_\pi$  in the first term. We examine in Tables II and III both  $\pi - {}^{40}\text{Ca}$  and  $\pi - {}^{208}\text{Pb}$  because  $Z\alpha$  is greater than  $\frac{1}{2}$  for Pb which means the Klein–Gordon, point–Coulomb solution (30) is pathological for  $l = 0$  (the finite-nucleus case is not).

Columns 2 and 3 in Table II indicate our numerical precision by comparing the computed and analytic results for the nonrelativistic Schrödinger equation (we know of no analytic results for the relativistic Schrödinger equation). We see that the numerical results are good out to the fifth decimal place, and that the computed  $2s$  and  $2p$  levels are degenerate (as well they should be) within numerical precision—even though the partial-wave potentials are quite different. Columns 3 and 4 in Table II and columns 2 and 3 in Table III indicate that relativistic effects are significant: 2% for  ${}^{40}\text{Ca}$ - $1s$ , 70% for  ${}^{208}\text{Pb}$ - $1s$ , and 48% for  ${}^{208}\text{Pb}$ - $2s$ . In contrast, columns 5 and 6 in Table II and columns 3 and 4 in Table III indicate that both the relativistic Schrödinger equation and the Klein–Gordon equation using the reduced mass, remove the degeneracy with  $l$  and include similar enough relativistic corrections for the differences to lie in the fourth significant figure. (The effect would be bigger for  $s$  states in Pb — if only they existed for the Klein–Gordon equation.)

Because these comparisons indicate that the inclusion of terms of higher order in the potential are important, and because the deeply bound states are hybrid nuclear-Coulomb, we conclude that ignoring the  $(V^{opt})^2$  term in the Klein–Gordon equation (3) may have a significant (probably several percent) effects upon the answers. This is consistent with the smaller effect found by Kwon and Tabakin [11] for the lower energy, and less relativistic,  $3d - 2p$  transition in  $K^- {}^{32}\text{S}$ .

## B. Experimental Shifts of Shallow States

The only adjustable parameters in our theory are the annihilation strengths  $B_0$  and  $C_0$ . Because our ultimate interest is the  $1s$  and  $2p$  levels (and because we want to avoid anomalies associated with the  $3d$  levels [24]), we fit the experimental energies and widths for the  $1s$  and  $2p$  levels in pionic  ${}^{16}\text{O}$  [25,26] and  $1s$  level in  ${}^{40}\text{Ca}$  [27,28], and determined

$$B_0 = (-0.074 + 0.067i)m_\pi^{-4}, \quad C_0 = (0.051 + 0.069i)m_\pi^{-6} \quad (32)$$

Since  $U^{(2)}$  provides the absorption in our model, the imaginary parts of  $B_0$  and  $C_0$  should have the most similarity to the work of others. The value for  $\text{Im } C_0$  in (32) is similar to those found in the coordinate space models, while the value for  $B_0$  is larger, although the momentum-space pionic atom calculation of Cieplý et al. [17] are more relevant. They fit the  $1s$  levels of  ${}^{12}\text{C}$  and  ${}^{16}\text{O}$ , and the  $2p$  levels of  ${}^{32}\text{S}$  and  ${}^{40}\text{Ca}$ , and find  $B_0 = (-0.093 + i0.042)m_\pi^{-4}$ ,  $C_0 = (-0.125 + 0.090i)m_\pi^{-6}$ . The differences probably reflect the differences in  $U^{(1)}$  and in the data fit.

We do not expect a theoretical potential to give the same level of agreement as a phenomenological potential whose many parameters have been determined in a global search. Nevertheless, in Table IV and Figure 1 we show a comparison between the strong interaction shifts predicted by our potential (the +’s) and various pionic atom data [25–30]. We see very good agreement for the heavier nuclei, good agreement for the lighter nuclei, and an incongruently large deviation for  ${}^{18}\text{O}$  (recall, we fit  $B_0$  and  $C_0$  to  ${}^{16}\text{O}$  and  ${}^{40}\text{Ca}$ ). In general, our level of agreement is comparable to the finite range, momentum space calculations of Cieplý et al. [17] — even though the potentials and calculational framework differ.

## C. Deep States

In Table V and Figure 2 we show the energies and widths of the deeply bound  $\pi - {}^{208}\text{Pb}$  states. The subscript  $EM$  denotes the inclusion of only electromagnetic interactions (Coulomb + vacuum polarization), *tot* the combined  $EM$

plus optical potentials, and  $r1$ ,  $r2$ , and  $r3$  the  $r$ -space calculations of Toki et al. [5], Nieves et al. [10], and of Konijn et al. [31]. We see that our calculated binding energies are slightly larger ( $\sim 7\%$ ) than those of Toki et al., Nieves et al., and Konijn et al. [31], and our widths are significantly larger: for the  $s$  states,  $\sim 20\%$  relative to Toki et al. [5] and  $\sim 200\%$  relative to Nieves et al. [10]; for the  $p$  and  $d$  states,  $\sim 50\%$  relative to Toki et al. and  $\sim 200 - 300\%$  relative to Nieves et al..

Because the differences increase with binding, the cause appears to be the energy dependences of the potentials, the different wave equations used, and the different extrapolations in the complex energy plane. Since the differences are much greater for  $\Gamma$  than  $\text{Re } E$ , the different annihilation potential has much to do with the differences (we use a finite range model, the others do not). We clearly are finding a much greater optical model dependence than  $(0.4, 15)\%$  in  $(\text{Re } E, \Gamma)$  found by Nieves et al. (possibly their  $7 - 75\%$  phenomenological renormalization of strengths reduced the model dependence they found). In our calculations, the vacuum polarization increases the binding by  $0.5\%$  and the width by  $2\%$ , which may be significant, but not compared to the model dependence.

To further understand the physics of the nonlocal optical potential and test the momentum space calculation, we have studied the wave functions of the deeply bound states. The momentum space wavefunctions are calculated via (25) and the coordinate space ones via the Bessel transform (29). In the top of Figure 3 we display the squared modulus of the momentum space wavefunction on a logarithmic scale, and in the bottom of the figure we display the coordinate space wavefunction  $\psi_l(r)$ , both for the  $1s$  state in Pb. We see in the comparison to the pure Coulomb wavefunction, that the optical potential introduces structures into the momentum space wavefunction similar to those present in the potential. These wavefunctions are similar in both shape and magnitude to those of Toki et al. [5], and should yield similar predictions when used in a DWIA calculation of the formation rate of the state.

Examination of the  $r$ -space wavefunction in the bottom of Figure 3, shows that the strong interaction repels the wavefunction out from the nuclear interior and that there is a node in  $\text{Re } \psi(r)$  even though this is a  $1s$  state. This node is a consequence of the existence of  $\text{Im } \psi_l(r)$  and the complex normalization constraint (26)-(28). The repulsion is also evident in Figure 4 where we plot the probability density [32]  $|u_l(r)|^2 \equiv |r\psi_l(r)|^2$  when there is only the EM potential (dashed curves) and when there is the EM plus nuclear potentials (solid curves). (The node is now hidden by the  $r^2$  multiplication.) We see in this figure the repulsion for the  $1s$ ,  $2p$  and  $2s$  states in Pb, while for  $3d$  and higher states there is an attraction. Similar results were found by Toki et al. [5].

While some repulsion (and the narrow widths) arise from the strong absorption of the wavefunction near the origin, the  $p$  wave repulsion occurs only for heavier nuclei. To understand this, we go back to the optical potential (14), and note that for nuclei which have  $Z \simeq N$ , the  $Zt^{\pi p} + Nt^{\pi n}$  term in the theoretical optical potential is attractive in  $p$  wave — as confirmed by the  $p$  level shifts in Table IV. Yet for nuclei which have  $N \gg Z$  like Pb, the  $t^{\pi n}$  term dominates and the  $p$  wave potential becomes repulsive. In the left part of Figure 5 we present  $V(p, p)$ , the diagonal parts of the momentum space potentials for the  $1s$  state in Pb and the  $2p$  state in  $^{40}\text{Ca}$ . The potential in this figure is clearly repulsive for the  $1s$  state in Pb and attractive for the  $2p$  state in Ca (although not shown, the  $2p$  potential in Pb is repulsive as expected). We also see in both cases that the imaginary part of the potential is absorptive.

#### D. Nuclear Bound States

We have found in our numerical searches that the optical potential is attractive enough to produce broad pion-nucleus resonances, but not attractive enough to produce pure nuclear bound states. We wondered how much stronger the optical potential is needed to support nuclear states, and so undertook a series of computations in which we progressively increased the strength of the optical potential while keeping the Coulomb potential constant. We found that the hybrid Coulomb-nuclear states eventually became nuclear ones, explicitly, for the range of strengths

$$V^{\text{coul}} + V^{\text{opt}} \leq V \leq V^{\text{coul}} + 15 V^{\text{opt}} \quad (33)$$

the complex binding energies found are:

$$-(0.4 + 0.001i) \text{ MeV} \leq E_{Ca} \leq -(5 + 5i) \text{ MeV} \quad (34)$$

$$-(7 + 0.4i) \text{ MeV} \leq E_{Pb} \leq -(22 + 13i) \text{ MeV} \quad (35)$$

In Figure 6 we present the probability density [32]  $|u_l(r)|^2$  for the  $1s$  state in  $\pi$ -Pb for varying optical potential strengths. We see the hybrid state slowly moving closer to the nucleus, until a transition takes place and at fifteen-fold strength the state is localized completely within the nucleus. When the optical potential is this strong, the state remain bound, for both Pb and Ca, even if the Coulomb potential is switched off.

The increase in binding and eventual nuclear state is expected for  $p$  states in Ca where the level shifts in Table IV are attractive. We were surprised, however, to find it for  $s$  states where the level shift is repulsive. At least for local

potentials, increasing the strength of the potential does not change its effect from repulsive to attractive. If we go back and look in the left part of Figure 5, we see that  $\text{Im } V_{OP}(p, p)$  always has the sign expected for an absorptive potential and that  $\text{Re } V_{OP}(p, p)$  appears attractive for the  $2p$  state in Ca and repulsive for the  $1s$  state in Pb. So this does not explain how we can get a  $1s$  nuclear state.

In an attempt to unravel the physics behind our nonlocal potential's  $1s$  bound states, we made use of our knowledge of the radial wavefunction  $u_l(r) \equiv r\psi_l(r)$  obtained via (25) and (29), to deduce an equivalent and local coordinate space potential. We assumed there is a  $V_{equiv}(r)$  which when used in a nonrelativistic Schrödinger equation produces this same  $u_l(r)$ :

$$V_{equiv}(r) = \frac{\hbar^2}{u_l(r)2\mu} \left[ \frac{d^2 u_l(r)}{dr^2} + \left( \frac{2\mu E}{\hbar^2} - \frac{l(l+1)}{r^2} \right) u_l(r) \right] \quad (36)$$

We evaluate the second derivative in (36) numerically using the central difference algorithm, and obtain the equivalent potential shown in the right hand side of Figure 5. While we do not expect such a  $V_{equiv}(r)$  to be the most physical of potentials, it is revealing, and the fact that the imaginary part of  $V_{equiv}(r)$  is always absorptive lends some confidence.

We see in the lower right-hand corner of Figure 5 that the real part of the  $V_{equiv}(r)$  for the normal strength  $2p$  state in Ca has a dominant, long range attraction — but also a short range repulsion. And since  $u_l(r)$  has no nodes, there is no division by zero in (36) to cause a sign change in  $V_{equiv}(r)$ . Yet we also find that the character of the potential changes dramatically as the nuclear bound state forms, with the potential acquiring an oscillation in the surface — much like the one expected from the  $\nabla \cdot \rho(r) \nabla$  term in the Ericson–Ericson potential. We find the bound state getting more bound, the wavefunction developing another node, and this showing up in the effective potential.

Much to our surprise, in the upper right-hand corner of Figure 5 we see that  $V_{equiv}(r)$  for the  $1s$  state in Pb has a central attraction in addition to a dominant, mid-range repulsion. This is true even at normal potential strength where the changeover in sign occurs close to the  $r$  value at which  $\text{Re } \psi_l(r)$  has a sign change in Figure 3. Accordingly, we now believe that the low energy pion optical potential has an  $s$  state repulsion on the outside of the nucleus and an attraction within. Furthermore, this shows how, as the nonlocal optical potential is made stronger, the effective attractive part increases in depth and eventually leads to a confined nuclear state.

#### IV. CONCLUSIONS

We have shown again [11,17] that pionic atom energies and wavefunctions can be calculated accurately in momentum space with a microscopic and nonlocal optical potential. Our particular potential includes effects from finite  $\pi N$  ranges in both the first and second order terms, covariant kinematics, Pauli exclusion, nucleon recoil, off-energy shell dynamics, and vacuum polarization. The Coulomb force is included exactly, and in our approach the energies and widths are determined by searching for the poles of the  $T$  matrix for the combined Coulomb plus nuclear potential. With present techniques we reproduce analytic results to five significant figures. Although computations in momentum space use more computer time than those in coordinate space, they can handle exactly various types of nonlocalities and can use theoretical results with fewer approximations; we also find them more elegant. Given modern computing techniques and machines, widespread momentum space applications are now practical as shown by our brief survey of levels throughout the periodic chart.

The focus of our calculations were the deeply bound ( $1s$ ,  $2s$ , and  $2p$ ) levels in lead which appear as hybrid Coulomb-nuclear states. Our calculations show these levels to be more bound and wider than reported previously [2,5,8]:  $\sim 7\%$  deeper,  $\sim 20 - 200\%$  wider  $s$  states, and  $\sim 50 - 300\%$  wider  $p$  and  $d$  states. The wavefunctions appear similar to those of Toki et al. [5] so we do not expect major changes in atomic formation rates. Most importantly, the states remain quasi-stable (nonoverlapping) and therefore are still experimentally observable. There may, however, be some changes needed in the experimental search for them.

The model dependence we have found appears to arise from our inclusion of energy dependences in the optical potential, complex energy extrapolations, and particularly our treatment of the finite-range annihilation term. The use of a relativistic wave equation is important for these states, and our use of the optical potential in a relativistic Schrödinger equation—as opposed to the approximate Klein-Gordon equation which ignores the quadratic  $V_{opt}^2$  term—may make some differences for these deeply bound states.

We view the major uncertainty in this work to be the description of pion annihilation. We use a quasi-deuteron absorption model, but it is not capable of predicting precise values for the annihilation strengths  $B_0$  and  $C_0$  at threshold, or their energy dependences below threshold. In addition, there are unknown isovector strengths to include for a nucleus such as lead, and they also appear to be accessible only phenomenologically and at threshold. A further concern than just the values of the strengths, is the simple assumption that the annihilation potential has  $\rho^2$

dependence; annihilation is a complicated process in which various numbers of nucleons enter, and the  $\rho^2$  dependence is only approximately true if there were only two.

We have also looked for pure nuclear bound states of pions at much deeper energies. We did not find any at normal densities and had to increase the strength of the nuclear potential at least eight-fold before any appeared. In the process of looking for these states we discovered that the real part of the effective local potential for a  $1s$  pion in Pb, while predominantly repulsive, has an inner attractive part. It is this attractive part which binds the pion within the nucleus as the potential strength is increased. Observing this dual character of the low energy potential experimentally would be fascinating, but difficult; measuring pion scattering from nuclei as a function of energy would not help much since the  $\pi N$  interaction itself is highly energy dependent. Likewise, the attractive  $p$  wave potential in Ca appears to have an inner part which is repulsive, and this too appears to be a new finding.

## ACKNOWLEDGMENTS

It is our pleasure to thank Eli Friedman for the conversations and assurances which stimulated the present study. We also wish to thank Iraj Afnan, Bill Kaufman, Anne Trudel, D. Frekers, Al Stetz, Carmen Garcia-Recio, and Avraham Gal for illuminating discussions. We gratefully acknowledge support from the U.S. Department of Energy under Grant DE-FG06-86ER40283 and the people at the National Institute for Nuclear Theory, Seattle for their hospitality during part of this work.

- 
- [1] R. Seki, Phys. Rev. C **5**, 1196 (1972); J.H. Koch, M.M. Sternheim, and J.F. Walker, Phys. Rev. C **5**, 381 (1972); T.E.O. Ericson and F. Schnock, Nucl. Phys. **B19**, 450 (1970).
  - [2] E. Friedman and G. Scoff, J. of Phys. G, **11**, (1985).
  - [3] S. Hirenzaki, T. Kajino, K.-I. Kubo, H. Toki, and I. Tanihata, Phys. Lett. B **194**, 20 (1987).
  - [4] H. Toki and T. Yamazaki, Phys. Lett. B **213**, 129 (1988).
  - [5] H. Toki, S. Hirenzaki, T. Yamazaki, and R.S. Hayano, Nucl. Phys. **A501**, 653 (1989).
  - [6] M. Iwasaki, A. Trudel, A. Celler, O. Käusser, T.S. Hayano, R. Helmer, R. Henderson, S. Hirenzaki, K.P. Jackson, Y. Kuno, N. Matsuoka, J. Mildenerger, C.A. Miller, H. Outa, H. Sakai, H. Toki, M. Vetterli, Y. Watanabe, T. Yamazaki, and S. Yen, Phys. Rev. C **43**, 1099 (1991).
  - [7] H. Toki, S. Hirenzaki and T. Yamazaki, Nucl. Phys. **A530**, 679 (1991).
  - [8] J. Nieves and E. Oset, Phys. Lett. **B282**, 24 (1992).
  - [9] W.B. Kaufmann, P.B. Siegel, and W.R. Gibbs, Arizona State University preprint, January 1992.
  - [10] J. Nieves, E. Oset and C. Garcia-Recio, Nucl. Phys. **A554**, 509 (1993).
  - [11] Y.R. Kwon and F. Tabakin, Phys. Rev. C **18**, 932 (1978); D.P. Heddle, Y.R. Kwon, and F. Tabakin, Comp. Phys. Comm. **38**, 71 (1985).
  - [12] R.H. Landau, S.C. Phatak, and F. Tabakin, Ann. Phys. **78**, 299 (1973); R.H. Landau, Comp. Phys. Comm. **28** 109 (1982).
  - [13] A. W. Thomas and R. H. Landau, Phys. Rep. **58**, No. 3, 121 (1980); R.H. Landau and A. W. Thomas, Nucl. Phys. **A302**(1978)461.
  - [14] L.L. Foldy and R.A. Krajcik, Phys. Rev/ Lett. **32**, 1025 (1974); F. Coester, Helv. Phys. Acta. **38**, 7, (1965).
  - [15] R.H. Landau, Quantum Mechanics II, J. Wiley, New York (1990).
  - [16] R.H. Landau, Phys. Rev. C **27**, 2191 (1983).
  - [17] A. Cieplý, M. Gmitro, R. Mach, S.S. Kamalov, Phys. Rev. C **44**, 713 (1991); M. Gmitro, S.S. Kamalov, and R. Mach, Phys. Rev. C **36**, 1105 (1987).
  - [18] G. Kalbermann, E. Friedman, A. Gal, and C.J. Batty, Nucl. Phys. **A503**, 632 (1989); C.J. Batty, E. Friedman, A. Gal, and G. Kalbermann, Nucl. Phys. **A535**, 548 (1991).
  - [19] J. Blomqvist, Nucl. Phys., **B48** 95 (1972).
  - [20] E. Friedman, personal communication.
  - [21] H. De Vries, C. W. De Jager, and C. De Vries, *Atomic Data and Nuclear Data Tables* **36**, 495 (1987).
  - [22] E. Hernández and A. Mondragon, Phys. Rev. C **29**, 722 (1984).
  - [23] H.A. Bethe and R. Jackiw, *Intermediate Quantum Mechanics*, W.A. Benjamin, Reading (1968).
  - [24] R. Seki, K. Masutani, M. Oka, and K. Yazaki, Phys. Lett. **97B**, 200 (1980); R. Seki and K. Masutani, Phys. Rev. C **27**, 2799 (1983); R. Seki, K. Masutani, and K. Yazaki, Phys. Rev. C **27**, 2817 (1983).
  - [25] I. Schwanner, R. Abela, G. Backenstoss, W. Kowald, P. Pavlopoulos, L. Tauscher, H.J. Weyer, P. Blüm, M. Dörr, W. Fetscher, D. Gotta, R. Guigas, H. Koch, H. Poth, G. Schmidt, and H. Ullrich, Phys. Lett. **96B**, 268 (1980).



- [26] G.De Chambrier, W. Beer, F.W.N. De Boer, K. Bos, A.I. Egorov, M. Eckhause, K.L. Giovanetti, P.F.A. Goudsmit, B. Jeckelmann, K.E. Kir'yanov, L.N. Kodurova, L. Lapina, H.J. Leisi, V.I. Marushenko, A.F. Mezentsev, A.A. Petrunin, A.G. Sergeev, A.I. Smirnov, G. Strassner, V.M. Suvorov, A. Vacchi, and D. Wieser, Nucl. Phys. **A442**, 637 (1985).
- [27] R.J. Powers, K.C. Wang, M.V. Hoehn, E.B. Shera, H.D. Wohlfahrt, and A.R. Kunselman, Nucl. Phys. **A336**, 475 (1980).
- [28] C.J. Batty, S.F. Biagi, E. Friedman, S.D. Hoath, J.D. Davies, G.J. Pyle, G.T.A. Squier, D.M. Asbury, and H. Guberman, Nucl. Phys. **A322**, 445 (1979).
- [29] C.J. Batty, S.F. Biagi, E. Friedman, S.D. Hoath, J.D. Davies, G.J. Pyle, G.T.A. Squire, D.M. Asbury, and M. Leon, Phys. Lett. **81B**, 165 (1979).
- [30] E. Friedman, H.J. Gils, H. Rebel, and Z. Majka, Phys. Rev. Lett. **41**, 1220 (1978).
- [31] J. Konijn, C.T.A.M. de Laat, A. Taal, and J.H. Koch, Nucl. Phys. **A519**, 773 (1990).
- [32] Because we use the Gamow state normalization (26)-(27), it can be argued that the proper probability density is  $(\text{Re } \psi_l(k))^2 - (\text{Im } \psi_l(k))^2$ . The difference is not significant for the present case.

FIG. 1. Comparison of optical potential predictions and measurements of shifts (top) and widths (bottom) for the indicated shallow levels of pionic atoms. Data are from references [25]- [30].

FIG. 2. Energy levels (top) and widths (bottom) of various deeply bound  $\pi^{-208}\text{Pb}$  states. The solid curves derive from the present p-space potential, the others from the r-space potentials of Toki et al. [5] and Nieves et al. [10].

FIG. 3. Momentum space wavefunction  $\psi_l(p)$  and coordinate space wavefunctions  $\psi_l(r)$  for  $\pi^- Pb$  1s state. Dashed curves derive from the EM potential alone, solid curves also contain the optical potential, and the dot-dashed curve shows  $\text{Im } \psi_l(r)$  for the total potential. A logarithmic scale is used for  $\psi_l(p)$  to show details of nuclear effect. In lower part of figure the exclusion of wavefunction from the nucleus of radius is  $\sim 7.1$  fm is evident as is the node introduced into the wavefunction.

FIG. 4. Probability density  $|u_l(r)|^2 \equiv |r\psi_l(r)|^2$  for the 1s, 2s, and 2p  $\pi^- Pb$  states. Dashed curves contain only the EM potential, solid curves EM plus optical potentials. The exclusion of wavefunction from the nucleus of radius is  $\sim 7.1$  fm is evident, although the node in the real part of the wavefunction at  $\sim 2.5$  evident in Figure 3 is not.

FIG. 5. The diagonal momentum space potentials  $V(p, p)$  (left) and equivalent local coordinate space potentials  $V_{equiv}(r)$  (right) for the 1s state in  $^{208}\text{Pb}$  (top) and the 2p state in  $^{40}\text{Ca}$  (bottom).

FIG. 6. Probability density  $|u_l(r)|^2 \equiv |r\psi_l(r)|^2$  of the 1s  $\pi^- Pb$  wave function arising from an optical potential increased, as in (33), by 1 (solid), 8 (dot-dashed), and 15 (dashed) times its normal value. The 15-fold increase leads to a nuclear bound state within the nucleus of radius  $\sim 7.1$  fm.

TABLE I. Parameters used in modified Wood-Saxon densities ( $R$  and  $a$  in fermis).

	$R_p$	$a_p$	$w_p$	$R_n$	$a_n$	$w_n$
$^{16}\text{O}$	2.608	0.513	-0.051	2.608	0.461	-0.051
$^{18}\text{O}$	2.634	0.513	0.0	2.72	0.447	0.0
$^{40}\text{Ca}$	3.669	0.584	-0.102	3.669	0.584	-0.102
$^{44}\text{Ca}$	3.70	0.55	0.0	3.82	0.505	0.0
$^{108}\text{Ag}$	5.32	0.52	0.0	5.47	0.473	0.0
$^{208}\text{Pb}$	6.624	0.549	0.0	6.624	0.549	0.0
$^{209}\text{Bi}$	6.609	0.545	0.0	6.88	0.5	0.0

TABLE II. Effect of different treatments of relativity on point Coulomb binding energies for  $\pi^- {}^{40}\text{Ca}$  atom. Compared are the analytic Schrödinger equation, the numeric Schrödinger equation, the relativistic Schrödinger equation, the Klein–Gordon equation with reduced mass, and the Klein–Gordon equation with pion mass. All energies in KeV.

$nl$	$E_{SE}(Anal)$	$E_{SE}(Num)$	$E_{RSE}$	$E_{KGE}(\mu)$	$E_{KGE}(m_\pi)$
$1s$	-1.4809	-1.4810	-1.5161	-1.5234	-1.5287
$2s$	-0.3702	-0.37025	-0.3761	-0.3772	-0.3785
$2p$	-0.3702	-0.37024	-0.3714	-0.3717	-0.3730

TABLE III. Effect of different treatments of relativity on point Coulomb binding energies (in MeV) for  $\pi^- {}^{208}\text{Pb}$  atom via Schrödinger equation, relativistic Schrödinger equation (numeric), and Klein–Gordon equation (which has no  $s$  states for  $Z\alpha > \frac{1}{2}$ ).

$nl$	$E_{SE}$	$E_{RSE}$	$E_{KGE}$
$1s$	-24.97	-42.53	n
$2s$	-6.243	-9.224	n
$2p$	-6.242	-6.584	-6.607
$3s$	-2.775	-3.659	n
$3p$	-2.775	-2.921	-2.929
$3d$	-2.774	-2.824	-2.829
$4s$	-1.562	-1.930	n
$4p$	-1.561	-1.632	-1.636
$4d$	-1.562	-1.592	-1.593
$4f$	-1.560	-1.574	-1.577

TABLE IV. Theoretical and experimental shifts and widths in KeV.

state	Ref	$Re E$	$\epsilon_{lpott}$	$\epsilon_{exp}$	$\Gamma_{lpott}$	$\Gamma_{exp}$
$1s {}^{16}\text{O}$	[25]	-219.98	-14.57	$-15.4 \pm 0.1$	8.14	$7.92 \pm 0.32$
$2p {}^{16}\text{O}$	[26]	-59.06	$13.4 \times 10^{-3}$	$14.8 \pm 1.6 \times 10^{-3}$	5.5	$6.8 \pm 0.4 \times 10^{-3}$
$1s {}^{18}\text{O}$	[25]	-215.76	-18.87	$-19.9 \pm 0.1$	7.40	$6.33 \pm 0.43$
$2p {}^{40}\text{Ca}$	[27,28]	-374.60	1.86	$1.86 \pm 0.08^a$	1.62	$1.62 \pm 0.11$
$2p {}^{44}\text{Ca}$	[29]	-374.78	1.92	$1.58 \pm 0.02$	1.84	$1.60 \pm 0.07$
$3d {}^{108}\text{Ag}$	[28]	-922.07	2.27	$1.97 \pm 0.03$	1.24	$1.41 \pm 0.05$
$4f {}^{208}\text{Pb}$	[29]	-1582.19	2.28	$1.67 \pm 0.02$	1.1	$1.17 \pm 0.05$
$4f {}^{209}\text{Bi}$	[30]	-1622.21	2.53	$1.83 \pm 0.06$	1.31	$1.24 \pm 0.14$

<sup>a</sup>Average experimental values.

TABLE V. Theoretical energies and widths in KeV for  $\pi^- - {}^{208}\text{Pb}$ . The subscripts  $r1$ ,  $r2$  and  $r3$  denote r-space calculations of Toki et al. [5], Nieves et al [10], and Konijn et al. [31].

$nl$	$E_{EM}$	$E_{lpott}$	$E_{r1}$	$E_{r2}$	$E_{r3}$	$\Gamma_{lpott}$	$\Gamma_{r1}$	$\Gamma_{r2}$	$\Gamma_{r3}$
$1s$	-12302	-7240	-6959	-6778	-6924	754	632	409	63
$2s$	-4492	-3043	-2962	-2902	-2954	208	183	140	13
$2p$	-5957	-5399	-5162	-5105	-5138	619	410	275	154
$3s$	-2262	-1682	-1642	-1613	-1633	88	78	65	5
$3p$	-2707	-2488	-2418	-2395	-2408	201	151	99	52
$3d$	-2831	-2916	-2854	-2858		125	91	56	
$4s$	-1352	-1067	-1045	-1026		45	40	35	
$4p$	-1538	-1436	-1408	-1394	-1394	90	71	46	24
$4d$	-1594	-1639	-1606	-1606		73	52	31	
$4f$	-1579	-1582	-1575	-1582		1.1	1.0	1.0	